LETTER TO THE EDITOR

Universal shape function for the double ionization cross section of negative ions by electron impact

Jan–Michael Rost† and Thomas Pattard‡

† Max-Planck-Institute for Physics of Complex Systems, Nöthnitzer Str. 38,
D-01187 Dresden, Germany
‡ Department of Physics, University of Tennessee, Knoxville, TN 37996–1200,
USA

Abstract. It is shown that recently measured cross sections for double ionization of negative ions (H^-, O^-, and C^-) possess a universal shape when plotted in suitable dimensionless units. The shape can be represented with a simple analytical function, following the same principles as it has been done in establishing a universal shape function for single ionization [Rost and Pattard 1997 Phys. Rev. A **55** R5]. Thereby, it is demonstrated that direct double ionization dominates the cross section for the targets considered.

In a complex ion such as O^- double ionization can proceed along different paths utilizing intermediate excited (autoionizing) states. How important are these indirect processes in comparison with direct double ionization (DDI) to describe total cross sections for double ionization (DI) of negative ions by electron impact? A calculation of a cross section from DDI processes alone compared to the experimental results could answer this question. However, neither such a calculation nor a full calculation exists for the published experimental cross sections involving the target ions H^- [1] and O^-, C^- [2]. Given this situation we have developed an alternative theoretical approach which has been applied successfully to the single ionization of atoms [3] and positively charged ions [4]. For these species we have established the existence and analytical form of a universal shape function for the cross section. In contrast to well known semi-empirical formulae (e.g. the Lotz formula [5]) our shape function uses the analytically known form of the cross section at high *and* low energies. Moreover, and this is crucial, the universal shape emerges only if the energy is measured from the ionization threshold I of the respective process, i.e. $E \geq 0$. (Usually, the energy is given in terms of the impact energy $E + I$).

The shape function itself is *parameter free*. It can be directly compared to the experimental cross section if the latter is plotted in dimensionless coordinates where the cross section y is written in terms of its maximum value $y = \sigma/\sigma_M$ and the energy is expressed in a scale which corresponds to the energy E_M where the maximum cross section appears, $x = E/E_M$. In practice, these two quantities σ_M and E_M may be viewed as fitting parameters and determined by a fit of the data to

$$\sigma(E) = \sigma_M f(E/E_M) \tag{1}$$

Table 1. Scaling parameters E_M, σ_M with uncertainties obtained by fitting the experimental cross sections from figure 2 with (1).

target	E_M (eV)	σ_M $(10^{-17} cm^2)$
H^-	36.0±0.6	0.935±0.008
O^-	100.3±0.6	5.33 ±0.02
C^-	57.0±1.0	7.44 ±0.07

where the shape function is given by

$$f(x) = x^\beta \left(\frac{\beta+1}{\beta x + 1} \right)^{\beta+1} . \tag{2}$$

The exponent β is the so called Wannier exponent which determines the energy variation of the cross section at low energies [6]. The corresponding power law behavior is included in (1) since $\sigma(E \to 0) \propto (E/E_M)^\beta$. For simplicity, the behavior for high energies is assumed to be classical, i.e. $1/E$ ignoring the logarithmic correction [3]. With these features, (1) has been designed to describe processes dominated by direct ionization (only in this case the specific power law applies - as does the single threshold I). Thereby, it is not important how many electrons have been ionized. (The number of ionized electrons enters (1) indirectly through the threshold exponent β which depends on the fragments and their charges.)

Therefore, apart from providing a useful, simple and universal parameterization for a large class of cross sections, (1) can be used to decide to which degree a cross section is dominated by direct processes. First of all, even without knowing a suitable parameterization of the cross section: if the shape of cross sections for rather different targets agrees one can conclude that their ionization is dominated by DDI. Secondly, knowing the final fragmented state of the system, one can usually calculate analytically or numerically the exponent β and a quantitative comparison with the shape function (1) becomes possible.

This is exactly our program for the rest of the paper. Firstly, we will demonstrate that to a good degree the DI cross sections for various targets (H^-, C^-, and O^-) possess a common shape when plotted in scaled coordinates as described above. From this observation we can conclude that the DI of these ions is dominated by direct double ionization. Secondly, we use the value $\beta = 2.83$ as calculated in [7] for three electrons and a positively charged ion in the continuum to construct the shape function (1) for our present needs.

We start from the cross sections for DI of H^- (double ionization potential $I = 14.35$eV), C^- ($I = 12.52$ eV) and O^- ($I = 15.08$ eV) as shown in figure 1. First, we replot these cross sections as a function of excess energy E in figure 2. Already included in this figure is a fit with (1) where the respective fitting parameters σ_M, E_M are listed in table 1. As a final step we scale the cross sections in terms of the respective maximum values from table 1. The result is shown in figure 3 and demonstrates the existence of a universal shape. Already at this point we may conclude that the process of DI for the investigated negative ions is dominated by DDI.

Proceeding further, we have overlaid in figure 3 the shape function from (2) with $\beta = 2.83$ (solid line). Obviously, this parameterization describes the universal shape well in the energy interval considered. Hence, we have provided additional evidence for the conjecture that double ionization of negative ions is dominated by direct processes.
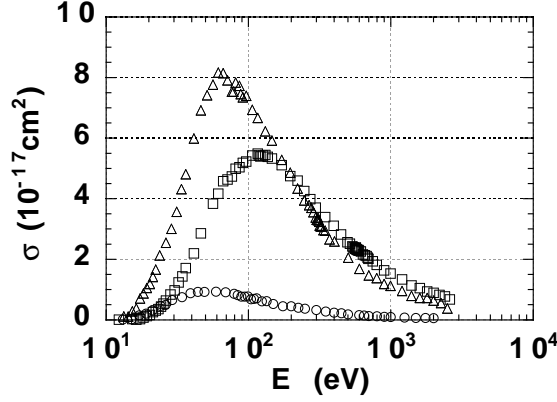
Figure 1. Double ionization cross sections for H^- (circles) [1], O^- (squares), and C^- (triangles) [2] as a function of electron impact energy $E + I$. The error bars do not exceed the size of the symbols.
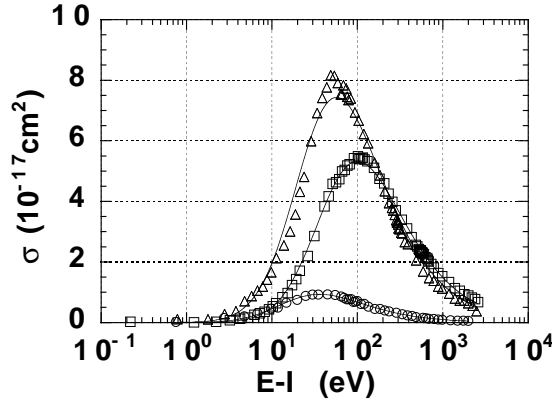

Figure 2. Double ionization cross sections for H^- (circles) [1], O^- (squares), and C^- (triangles) [2] as a function of excess energy E. In addition, the fits according to (1) are shown with solid lines.

This is in agreement with the conclusion reached in [2], although this conclusion was somewhat weakened by the poor agreement with existing semiempirical formulae. In one respect we arrive at a different result: The Wannier-threshold behavior with the exponent derived by Klar and Schlecht [7] fits well into our description of the ionization cross sections. In contrast, a fit with (1) where $\beta = 1.3$ as suggested in [2] agrees only poorly with the experimental cross sections. It seems that without a shape function valid over a larger range of energy the determination of the threshold exponent β from fitting a cross section of the form $\sigma \propto E^\beta$ to the data of figure 1 is rather unreliable. Similar situations have been encountered for other collisional systems, in particular with positron impact.

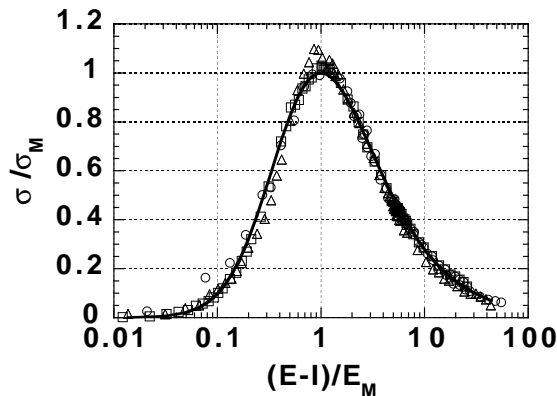We conclude that due to the dominance of direct double ionization processes the

Figure 3. Double ionization cross sections for H^- (circles) [1], O^- (squares), and C^- (triangles) [2] in terms of the maximum values E_M, σ_M. In addition the shape function (2) is shown with a solid line.

overall shape of DI cross sections is a rather robust function which is not strongly influenced by details of the collision dynamics different for each scattering system. From the quality of the fit, one may speculate that among the systems taken into account here, C^- exhibits the strongest influence of indirect DI processes (see table 1 and figures 2 and 3). However, even in this case the overall shape of the DI cross section is still well reproduced by the shape function based only on DDI processes, taking into consideration that the scale of the ordinate in our figures is linear in contrast to the usual logarithmic representations of cross sections.

References

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